

the formula of Perard,³ which differs appreciably from that of Meggers and Peters in the visible and ultraviolet. Perard's equation, rewritten for the special case of normal pressure and 15°C, in units to correspond with the equation above, is

$$(n-1)10^7 = 2728.13 + 14.038/(\lambda^2 \times 10^{-8}) + 0.3367/(\lambda^4 \times 10^{-16}).$$

If a table of vacuum wave numbers were based on this formula it would show systematic differences from Kayser's table, amounting to about 1 part in 725,000 in the ultraviolet but negligible in the infrared.

It will be noted that the correction to be applied to the inverted table of Kayser is very

³ Perard, *J. de Phys. et le Rad.* 6, 217 (1925).

small between $\lambda 10,000$ and the present limit of photography, $\lambda 12,500$, at which point it reaches a magnitude of 1 part in 800,000. For lines whose wave-length is not known with such accuracy the correction may be ignored. Farther in the infrared the relative importance of the correction increases more rapidly. The last entry in the table is of low weight. Observations made in moist air for spectral regions close to the important absorption bands of water vapor or of CO₂ may possibly be affected by anomalies in the index of refraction which are not represented in the equation used for extrapolation.

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The Kinetic Energy of Polyatomic Molecules

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The Lagrangian and Hamiltonian expressions for the kinetic energy of a system of N particles are obtained in such a form that the rotational, vibrational and coupling terms may be distinguished. The principal axes of inertia are used to define rotation. The ordinary moments of

inertia appear in the Lagrangian kinetic energy but these are replaced by other functions of the radii of gyration in the Hamiltonian. This throws doubt upon all molecular configurations assigned on the basis of empirical values of the moments of inertia.

INTRODUCTION

IT is proposed to derive the expression for the kinetic energy of a polyatomic molecule, considered as a system of N particles, in such a form that its rotational, vibrational and coupling terms may be distinguished.

I. THE PRINCIPAL AXIS TRANSFORMATION; COORDINATES

It is no loss of generality to suppose the center of mass of the molecule to be at rest, so that its configuration is completely specified by $n = N - 1$ vectors \mathbf{R}_α , $\alpha = 1, 2, 3, \dots, n$. It is convenient to choose these vectors so that two conditions are fulfilled: (1) the kinetic energy T is given by

$$2T = \mu \sum_{\alpha} (d\mathbf{R}_\alpha/dt)^2 \quad (1)$$

and (2) any other vector dimension \mathbf{X} of the

configuration is given by

$$\mathbf{X} = \sum_{\alpha} X_{\alpha} \mathbf{R}_{\alpha}, \quad (2)$$

where the X_{α} are independent of the \mathbf{R}_{α} . These two conditions may always be satisfied and do not determine the vectors \mathbf{R}_{α} uniquely. In fact the constant μ is quite arbitrary and the vectors \mathbf{R}_{α} may be replaced by any n linear functions of themselves, provided that the coefficients of these functions form an orthogonal matrix and are independent of the \mathbf{R}_{α} . It is convenient to set $\mu = 1$ for general considerations.

The length of the vector \mathbf{X} is given by the quadratic form

$$\mathbf{X}^2 = \sum_{\alpha} \sum_{\beta} X_{\alpha} X_{\beta} \mathbf{R}_{\alpha} \cdot \mathbf{R}_{\beta}. \quad (3)$$

The matrix of this form is also the matrix of the Gram¹ determinant of the vectors \mathbf{R}_{α} . It is known,

¹ Courant-Hilbert, *Methoden der mathematischen Physik*, 1st Ed., p. 20.

or may easily be shown, that this matrix possesses exactly as many non-zero characteristic values as there are linearly independent vectors among the \mathbf{R}_α . It is therefore evident that when $n \geq 3$, the quadratic form will have three characteristic values which do not vanish identically and $n-3$ which do vanish identically. The triatomic molecule for which $n=2$ thus occupies an exceptional position in the theory; to avoid confusion, it will be discussed separately in Part IV.

With this understanding, let r_1^2, r_2^2, r_3^2 be the non-vanishing characteristic values of the form \mathbf{X}^2 and set $r_4^2 = \dots = r_n^2 = 0$. Then it is known from the general theory of quadratic forms that an orthogonal matrix $c_{\gamma\alpha}$ exists, such that

$$\sum_{\alpha} c_{\gamma\alpha} \mathbf{R}_\alpha \cdot \mathbf{R}_\beta = r_\gamma^2 c_{\gamma\beta}. \quad (4)$$

The conditions for the orthogonality of the matrix are

$$\sum_{\beta} c_{\alpha\beta} c_{\gamma\beta} = \delta_{\alpha\gamma}, \quad (5.1)$$

$$\sum_{\beta} c_{\beta\alpha} c_{\beta\gamma} = \delta_{\alpha\gamma}. \quad (5.2)$$

Its elements will, of course, be functions of the \mathbf{R}_α , which distinguishes it from the orthogonal matrices discussed above.

If the n quantities defined by

$$X_\alpha = \sum_{\gamma} x_\gamma c_{\gamma\alpha} \quad \text{or} \quad x_\alpha = \sum_{\gamma} c_{\alpha\gamma} X_\gamma \quad (6)$$

are substituted into Eq. (3), it becomes

$$\mathbf{X}^2 = \sum_{\gamma} r_\gamma^2 x_\gamma^2 = r_1^2 x_1^2 + r_2^2 x_2^2 + r_3^2 x_3^2. \quad (7)$$

Again, in distinction to the X_α , the x_γ and r_γ are functions of the \mathbf{R}_α . To avoid repetition, it is convenient to introduce the convention that the Latin indices i, j, k have the range 1, 2, 3, while the Greek indices $\alpha, \beta, \gamma, \delta$ have the range 1, 2, \dots, n . Next consider the three vectors \mathbf{a}_i , defined by

$$r_i \mathbf{a}_i = \sum_{\alpha} c_{i\alpha} \mathbf{R}_\alpha. \quad (8)$$

It is easily seen that they are mutually perpendicular and of unit length, since

$$\begin{aligned} r_i r_j \mathbf{a}_i \cdot \mathbf{a}_j &= \sum_{\alpha} \sum_{\beta} c_{i\alpha} c_{j\beta} \mathbf{R}_\alpha \cdot \mathbf{R}_\beta \\ &= \sum_{\beta} r_i^2 c_{i\beta} c_{j\beta} && \text{by Eq. (4),} \\ &= r_i^2 \delta_{ij} && \text{by Eq. (5.1).} \end{aligned}$$

These vectors may be used to define a rotating set of coordinate axes, to which the components

of the vectors \mathbf{R}_α may be referred. From Eq. (8) it follows that

$$r_i \mathbf{a}_i \cdot \mathbf{R}_\beta = \sum_{\alpha} c_{i\alpha} \mathbf{R}_\alpha \cdot \mathbf{R}_\beta = r_i^2 c_{i\beta},$$

whence

$$\mathbf{R}_\alpha = \sum_i \mathbf{a}_i r_i c_{i\alpha}. \quad (9)$$

It is advantageous to choose the generalized coordinates in such a manner that they correspond to the various elements distinguishable on the right side of Eq. (9). Thus the three quantities r_1, r_2, r_3 may themselves be chosen as three of the $3n$ coordinates. The axes \mathbf{a}_i may be specified by three Eulerian angles according to the usual formulae ($\mathbf{i}, \mathbf{j}, \mathbf{k}$ are three stationary unit vectors):

$$\begin{aligned} \mathbf{k} \cdot \mathbf{a}_1 &= -\sin \beta \cos \gamma, & \mathbf{a}_3 \cdot \mathbf{i} &= \sin \beta \cos \alpha, \\ \mathbf{k} \cdot \mathbf{a}_2 &= \sin \beta \sin \gamma, & \mathbf{a}_3 \cdot \mathbf{j} &= \sin \beta \sin \alpha, \\ & & \mathbf{k} \cdot \mathbf{a}_3 &= \cos \beta. \end{aligned} \quad (10)$$

The $3n$ quantities $c_{i\alpha}$ are related by six equations (Eq. (5.1)) so that they can all be specified as functions of $3n-6$ dimensionless quantities q_κ . Thus the total of $3n$ is made up of three different kinds of coordinates.

The further convention that the index κ has the range 1, 2, $\dots, 3n-6$, is hereby introduced.

II. THE LAGRANGIAN FORM OF THE KINETIC ENERGY

As the Lagrangian form of the kinetic energy depends on the time derivatives of the coordinates, it will be necessary to express $d\mathbf{R}_\alpha/dt$ in terms of these. To avoid complicated expressions, it is convenient to define certain auxiliary quantities which are linear functions of these derivatives. The first of these is the ordinary angular velocity vector, $\boldsymbol{\omega}$, defined by

$$d\mathbf{a}_i/dt = \boldsymbol{\omega} \times \mathbf{a}_i, \quad (11)$$

or more explicitly by

$$\begin{aligned} \boldsymbol{\omega} &= \sum_i \omega_i \mathbf{a}_i \\ &= \mathbf{a}_1(-\dot{\alpha} \sin \beta \cos \gamma + \dot{\beta} \sin \gamma) \\ &\quad + \mathbf{a}_2(\dot{\alpha} \sin \beta \sin \gamma + \dot{\beta} \cos \gamma) \\ &\quad + \mathbf{a}_3(\dot{\alpha} \cos \beta + \dot{\gamma}). \end{aligned} \quad (11.1)$$

The second set of auxiliary quantities are matrices defined by

$$\Omega_{\beta\gamma} = \sum_{\alpha} c_{\alpha\beta} \dot{c}_{\alpha\gamma}, \quad \omega_{\beta\gamma} = \sum_{\alpha} \dot{c}_{\beta\alpha} c_{\gamma\alpha}. \quad (12)$$

On differentiating Eq. (5) it appears that both these matrices are skew-symmetric; both are linear functions of the \dot{q}_k , so that, e.g.,

$$\omega_{\beta\gamma} = \sum_{\kappa} \omega_{\beta\gamma,\kappa} \dot{q}_{\kappa}, \quad (13)$$

where the $\omega_{\beta\gamma,\kappa}$ are functions of the q_{κ} only. Combining Eq. (5) with Eq. (12), it follows that

$$\sum_{\beta} c_{\alpha\beta} \Omega_{\beta\gamma} = \dot{c}_{\alpha\gamma} = \sum_{\beta} \omega_{\alpha\beta} c_{\beta\gamma}, \quad (14.1)$$

and hence that

$$\omega_{\alpha\delta} = \sum_{\beta} \sum_{\gamma} c_{\alpha\beta} \Omega_{\beta\gamma} c_{\delta\gamma}. \quad (14.2)$$

The matrices $\Omega_{\beta\gamma}$ and $\omega_{\beta\gamma}$ are the n -dimensional analogues of the angular velocity vector and the q_{κ} are the analogues of the Eulerian angles. The elements $\Omega_{\beta\gamma}$ are the components of the n -dimensional angular velocity relative to "moving" axes (system of the X_{α}) and the $\omega_{\beta\gamma}$ are the components of the same quantity relative to "fixed" axes (system of the x_{α}).

The use of Eqs. (11) and (14.1) now makes it possible to write

$$d\mathbf{R}_{\alpha}/dt = \boldsymbol{\omega} \times \mathbf{R}_{\alpha} + \sum_i \mathbf{a}_i \dot{r}_i c_{i\alpha} + \sum_{\beta} \mathbf{R}_{\beta} \Omega_{\beta\alpha}. \quad (15)$$

For temporary convenience, call the three terms of this expression \mathbf{A}_{α} , \mathbf{B}_{α} , \mathbf{C}_{α} ; then the kinetic energy is

$$2T = \sum_{\alpha} [(\mathbf{A}_{\alpha}^2 + \mathbf{B}_{\alpha}^2 + \mathbf{C}_{\alpha}^2) + 2(\mathbf{A}_{\alpha} \cdot \mathbf{B}_{\alpha} + \mathbf{B}_{\alpha} \cdot \mathbf{C}_{\alpha} + \mathbf{C}_{\alpha} \cdot \mathbf{A}_{\alpha})]. \quad (16)$$

The six terms of this sum will be given separate consideration; the first is

$$\begin{aligned} \sum_{\alpha} \mathbf{A}_{\alpha}^2 &= \sum_{\alpha} (\boldsymbol{\omega} \times \mathbf{R}_{\alpha})^2 = \sum_{\alpha} [\boldsymbol{\omega}^2 \mathbf{R}_{\alpha}^2 - (\boldsymbol{\omega} \cdot \mathbf{R}_{\alpha})^2] \\ &= \sum_{\alpha} \sum_i \sum_j [\omega_i^2 r_j^2 c_{j\alpha}^2 - \omega_i r_i c_{i\alpha} \omega_j r_j c_{j\alpha}] \end{aligned}$$

by Eqs. (9) and (11.1);

$$= \sum_i \sum_j [\omega_i^2 r_j^2 - \omega_i^2 r_i^2 \delta_{ij}]$$

by Eq. (5.1), so that

$$\sum_{\alpha} \mathbf{A}_{\alpha}^2 = \omega_1^2 (r_2^2 + r_3^2) + \omega_2^2 (r_3^2 + r_1^2) + \omega_3^2 (r_1^2 + r_2^2).$$

The second term is

$$\sum_{\alpha} \mathbf{B}_{\alpha}^2 = \sum_{\alpha} \sum_i \dot{r}_i^2 c_{i\alpha}^2 = \sum_i \dot{r}_i^2$$

by Eq. (5.1) again; the third term is

$$\begin{aligned} \sum_{\alpha} \mathbf{C}_{\alpha}^2 &= \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \mathbf{R}_{\beta} \cdot \mathbf{R}_{\gamma} \Omega_{\beta\alpha} \Omega_{\gamma\alpha} \\ &= \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \sum_i r_i^2 c_{i\beta} c_{i\gamma} \Omega_{\beta\alpha} \Omega_{\gamma\alpha} \end{aligned}$$

by Eq. (9), whence

$$\sum_{\alpha} \mathbf{C}_{\alpha}^2 = \sum_{\alpha} \sum_i r_i^2 \omega_{i\alpha}^2$$

by Eqs. (14.1) and (5.1). The fourth and fifth terms vanish, since

$$\begin{aligned} \sum_{\alpha} \mathbf{A}_{\alpha} \cdot \mathbf{B}_{\alpha} &= \sum_{\alpha} \sum_i \boldsymbol{\omega} \times \mathbf{R}_{\alpha} \cdot \mathbf{a}_i \dot{r}_i c_{i\alpha} \\ &= \boldsymbol{\omega} \cdot \sum_{\alpha} \sum_i \mathbf{R}_{\alpha} \times \mathbf{a}_i \dot{r}_i c_{i\alpha} \end{aligned}$$

and

$$\sum_{\alpha} \mathbf{R}_{\alpha} \times \mathbf{a}_1 c_{1\alpha} = \sum_{\alpha} (\mathbf{a}_3 r_2 c_{2\alpha} - \alpha_2 r_3 c_{3\alpha}) c_{1\alpha} = 0$$

by Eq. (5.1); also

$$\begin{aligned} \sum_{\alpha} \mathbf{B}_{\alpha} \cdot \mathbf{C}_{\alpha} &= \sum_{\alpha} \sum_{\beta} \sum_i \mathbf{a}_i \cdot \mathbf{R}_{\beta} \dot{r}_i c_{i\alpha} \Omega_{\beta\alpha} \\ &= \sum_{\alpha} \sum_{\beta} \sum_i \dot{r}_i r_i c_{i\alpha} c_{i\beta} \Omega_{\beta\alpha} \end{aligned}$$

by Eq. (9),

$$= \sum_i \dot{r}_i r_i \omega_{ii} = 0$$

by Eq. (14.2). The last term does not vanish:

$$\sum_{\alpha} \mathbf{C}_{\alpha} \cdot \mathbf{A}_{\alpha} = \boldsymbol{\omega} \cdot [\sum_{\alpha} \sum_{\beta} \mathbf{R}_{\alpha} \times \mathbf{R}_{\beta} \Omega_{\beta\alpha}];$$

since the \mathbf{a}_1 -component of $\mathbf{R}_{\alpha} \times \mathbf{R}_{\beta}$ is

$$r_2 r_3 (c_{2\alpha} c_{3\beta} - c_{3\alpha} c_{2\beta})$$

(by Eq. (9)), it is easily seen upon referring to Eq. (14.2) that

$$\sum_{\alpha} \mathbf{C}_{\alpha} \cdot \mathbf{A}_{\alpha} = -2(r_2 r_3 \omega_1 \omega_{23} + r_3 r_1 \omega_2 \omega_{31} + r_1 r_2 \omega_3 \omega_{12}).$$

Combining all these results according to Eq. (16), the Lagrangian form of the kinetic energy appears:

$$\begin{aligned} 2T &= \dot{r}_1^2 + \dot{r}_2^2 + \dot{r}_3^2 + \omega_1^2 (r_2^2 + r_3^2) \\ &\quad + \omega_2^2 (r_3^2 + r_1^2) + \omega_3^2 (r_1^2 + r_2^2) - 4r_2 r_3 \omega_1 \omega_{23} \\ &\quad - 4r_3 r_1 \omega_2 \omega_{31} - 4r_1 r_2 \omega_3 \omega_{12} \\ &\quad + \sum_{\alpha} (r_1^2 \omega_{1\alpha}^2 + r_2^2 \omega_{2\alpha}^2 + r_3^2 \omega_{3\alpha}^2). \quad (17) \end{aligned}$$

From the form of this expression, it is possible to draw certain conclusions as to the significance of the coordinates which were introduced at the end of Part I. Since there are no terms containing $\omega_1 \omega_2$, etc., it follows that the vectors \mathbf{a}_i are along the principal axes of inertia of the instantaneous

configuration of the N particles; this justifies the title of Part I. From the mode of calculation it also follows that

$$A_1 = r_2^2 + r_3^2, \quad \text{etc.}, \quad (18)$$

are the three Eulerian moments of inertia. The three coordinates r_1, r_2, r_3 may therefore be called the radii of gyration of the instantaneous configuration, although this deviates slightly from the usual definition of the term.

III. THE HAMILTONIAN FORM OF THE KINETIC ENERGY

Eq. (17) may be rearranged into the form

$$\begin{aligned} 2T = & \dot{r}_1^2 + \dot{r}_2^2 + \dot{r}_3^2 \\ & + (r_2\omega_1 - r_3\omega_{23})^2 + (r_3\omega_1 - r_2\omega_{23})^2 \\ & + (r_3\omega_2 - r_1\omega_{31})^2 + (r_1\omega_2 - r_3\omega_{31})^2 \\ & + (r_1\omega_3 - r_2\omega_{12})^2 + (r_2\omega_3 - r_1\omega_{12})^2 \\ & + \sum_{\alpha=4}^n (r_1^2\omega_{1\alpha}^2 + r_2^2\omega_{2\alpha}^2 + r_3^2\omega_{3\alpha}^2), \quad (17.1) \end{aligned}$$

which is more convenient for the calculation of the momenta. In case $n=3$ (tetra-atomic molecule), the residual sum on the last line vanishes. On calculating the momenta in the usual manner, one finds that

$$P_i = \partial T / \partial \dot{r}_i = \dot{r}_i \quad (19)$$

and on referring to Eq. (13):

$$\begin{aligned} p_{\kappa} = & \partial T / \partial \dot{q}_{\kappa} \\ = & \omega_{23, \kappa} [-r_3(r_2\omega_1 - r_3\omega_{23}) - r_2(r_3\omega_1 - r_2\omega_{23})] \\ & + \omega_{31, \kappa} [-r_1(r_3\omega_2 - r_1\omega_{31}) - r_3(r_1\omega_2 - r_3\omega_{31})] \\ & + \omega_{12, \kappa} [-r_2(r_1\omega_3 - r_2\omega_{12}) - r_1(r_2\omega_3 - r_1\omega_{12})] \\ & + \sum_{\alpha=4}^n (r_1^2\omega_{1\alpha}\omega_{1\alpha, \kappa} + r_2^2\omega_{2\alpha}\omega_{2\alpha, \kappa} \\ & \quad + r_3^2\omega_{3\alpha}\omega_{3\alpha, \kappa}). \quad (20) \end{aligned}$$

These are $3n-6$ equations; the $3n-9$ quantities $r_i^2\omega_{i\alpha}$ and the three square brackets may be treated as unknowns and expressed as linear functions of the p_{κ} upon solution of the equations. Supposing this to have been accomplished, it follows that

$$r_i^2\omega_{i\alpha} = N_{i\alpha} = \sum_{\kappa} N_{i\alpha, \kappa} p_{\kappa}, \quad \alpha = 4 \cdots 3n-6, \quad (21.1)$$

where the $N_{i\alpha, \kappa}$ are functions of the q_{κ} only.

Similarly

$$\begin{aligned} -r_3(r_2\omega_1 - r_3\omega_{23}) - r_2(r_3\omega_1 - r_2\omega_{23}) & = N_{23}, \\ N_{23} & = \sum_{\kappa} N_{23, \kappa} p_{\kappa}, \quad \text{etc.} \quad (21.2) \end{aligned}$$

On dealing with the ordinary angular velocity in the same manner as has just been done with the n -dimensional one, it follows that

$$r_2(r_2\omega_1 - r_3\omega_{23}) + r_3(r_3\omega_1 - r_2\omega_{23}) = M_1, \quad \text{etc.}, \quad (22)$$

where²

$$\begin{aligned} M_1 & = \cos \gamma (-p_{\alpha} + p_{\gamma} \cos \beta) / \sin \beta + p_{\beta} \sin \gamma, \\ M_2 & = -\sin \gamma (-p_{\alpha} + p_{\gamma} \cos \beta) / \sin \beta + p_{\beta} \cos \gamma, \\ M_3 & = p_{\gamma}. \quad (23) \end{aligned}$$

In passing, it may be remarked that the total angular momentum (three dimensional) of the system can be shown to be

$$\mathbf{M} = \mathbf{a}_1 M_1 + \mathbf{a}_2 M_2 + \mathbf{a}_3 M_3 \quad (24)$$

in accord with the well-known formula. On solving Eqs. (21.2) and (22) for the two parentheses, one sees that

$$\begin{aligned} r_2\omega_1 - r_3\omega_{23} & = (r_2 M_1 - r_3 N_{23}) / (r_2^2 - r_3^2), \\ r_3\omega_1 - r_2\omega_{23} & = (r_3 M_1 - r_2 N_{23}) / (r_3^2 - r_2^2), \quad \text{etc.} \quad (25) \end{aligned}$$

On substituting Eqs. (19), (21.1) and (25) into Eq. (17.1), the Hamiltonian form appears:

$$\begin{aligned} 2T = & P_1^2 + P_2^2 + P_3^2 \\ & + M_1^2/B_1 + M_2^2/B_2 + M_3^2/B_3 \\ & - 2(M_1 N_{23}/C_1 + M_2 N_{31}/C_2 + M_3 N_{12}/C_3) \\ & + N_{23}^2/B_1 + N_{31}^2/B_2 + N_{12}^2/B_3 \\ & + \sum_{\alpha=4}^n (N_{1\alpha}^2/r_1^2 + N_{2\alpha}^2/r_2^2 + N_{3\alpha}^2/r_3^2), \quad (26) \end{aligned}$$

where

$$B_1 = (r_2^2 - r_3^2)^2 / (r_2^2 + r_3^2), \quad \text{etc.}, \quad (27.1)$$

$$C_1 = (r_2^2 - r_3^2)^2 / (2r_2 r_3), \quad \text{etc.} \quad (27.2)$$

The first, fourth and fifth lines of Eq. (26) represent the vibrational kinetic energy; the rotational is given by the second and the coupling by the third. It will be noted that the Eulerian moments of inertia A_i , do not enter into the

² The indices α, β, γ in Eq. (23) refer to the Eulerian angles and are not the same as those used in the n -dimensional geometry.

second line as expected, but are replaced by the coefficients B_i .

In order to set up the wave equation, it is also necessary to know the element of volume in configuration space. This is proportional to the square root of the discriminant of the Lagrangian form³ and a simple calculation shows that

$$d\tau = (r_2^2 - r_3^2)(r_3^2 - r_1^2)(r_1^2 - r_2^2)(r_1 r_2 r_3)^{n-3} \sin \beta J(q_\kappa) dr_1 dr_2 dr_3 d\alpha d\beta d\gamma dq_1 \cdots dq_{3n-6}, \quad (28)$$

where $J(q_\kappa)$ is the determinant of $(3n-6)$ th order whose κ -th row is

$$\omega_{23, \kappa}, \omega_{31, \kappa}, \omega_{12, \kappa}, \omega_{14, \kappa} \cdots \omega_{3n, \kappa}. \quad (29)$$

IV. THE TRIATOMIC CASE

The investigation of the triatomic case parallels the preceding in all essential respects. Since $n=2$, there are only two vectors \mathbf{R}_1 and \mathbf{R}_2 , which satisfy the same conditions (Eqs. (1) and (2)) as before. The orthogonal transformation of Eq. (6) is introduced in the same manner but can be written out explicitly:

$$\begin{aligned} X_1 &= x_1 \cos q + x_2 \sin q, \\ X_2 &= -x_1 \sin q + x_2 \cos q, \end{aligned} \quad (6.3)$$

where the parameter q is the sole representative of the coordinates q_κ . There are only two radii of gyration, r_1 and r_2 , and only two unit vectors can be defined:

$$\begin{aligned} r_1 \mathbf{a}_1 &= \mathbf{R}_1 \cos q - \mathbf{R}_2 \sin q, \\ r_2 \mathbf{a}_2 &= \mathbf{R}_1 \sin q + \mathbf{R}_2 \cos q, \end{aligned} \quad (8.3)$$

so that the third must be defined by

³ A. Sommerfeld, *Wellenmechanischer Ergänzungsband*, pp. 148, 152; A. Landé, *Handbuch der Physik*, XX, p. 330.

$$\mathbf{a}_3 = \mathbf{a}_1 \times \mathbf{a}_2.$$

Eqs. (8.3), when solved for \mathbf{R}_1 and \mathbf{R}_2 become

$$\begin{aligned} \mathbf{R}_1 &= \mathbf{a}_1 r_1 \cos q + \mathbf{a}_2 r_2 \sin q, \\ \mathbf{R}_2 &= -\mathbf{a}_1 r_1 \sin q + \mathbf{a}_2 r_2 \cos q. \end{aligned} \quad (9.3)$$

The Eulerian angles are defined as before by Eq. (10) and complete the total of six coordinates.

The n -dimensional angular velocities are here one-dimensional and need not be discussed explicitly. The kinetic energy is readily found to be

$$\begin{aligned} 2T &= \dot{r}_1^2 + \dot{r}_2^2 + \omega_1^2 r_2^2 + \omega_2^2 r_1^2 + \omega_3^2 (r_1^2 + r_2^2) \\ &\quad - 4r_1 r_2 \omega_3 \dot{q} + (r_1^2 + r_2^2) \dot{q}^2. \end{aligned} \quad (17.3)$$

The Hamiltonian form is readily derived from this by the same methods as before and is

$$\begin{aligned} 2T &= P_1^2 + P_2^2 + M_1^2/r_2^2 + M_2^2/r_1^2 \\ &\quad + M_3^2/B_3 + 2M_3 p/C_3 + p^2/B_3. \end{aligned} \quad (26.3)$$

The element of volume is

$$d\tau = r_1 r_2 (r_1^2 - r_2^2) \sin \beta dr_1 dr_2 d\alpha d\beta d\gamma dq. \quad (27.3)$$

A more extended investigation of the triatomic molecule was begun prior to the investigation reported in this paper. On encountering the unexpected form of the coefficient of M_3^2 in Eq. (26.3) it seemed advisable to examine the general case before continuing. The present results throw doubt on molecular configurations previously assigned on the basis of empirical values of the moments of inertia. These empirical values are presumably closer to the equilibrium values of the B_i than the A_i , as has been supposed.